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Trying 3106016892...Open

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LOGINID:ssspta1612BXR
PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2	Dec 17	The CA Lexicon available in the CAPLUS and CA files
NEWS	3	Feb 06	Engineering Information Encompass files have new names
NEWS	4	Feb 16	TOXLINE no longer being updated
NEWS	5	Apr 23	Search Derwent WPINDEX by chemical structure
NEWS	6	Apr 23	PRE-1967 REFERENCES NOW SEARCHABLE IN CAPLUS AND CA
NEWS	7	May 07	DGENE Reload
NEWS	8	Jun 20	Published patent applications (A1) are now in USPATFULL
NEWS	9	JUL 13	New SDI alert frequency now available in Derwent's DWPI and DPCI

NEWS EXPRESS	July 11 CURRENT WINDOWS VERSION IS V6.0b, CURRENT MACINTOSH VERSION IS V5.0C (ENG) AND V5.0JB (JP), AND CURRENT DISCOVER FILE IS DATED 06 APRIL 2001
NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS INTER	General Internet Information
NEWS LOGIN	Welcome Banner and News Items
NEWS PHONE	Direct Dial and Telecommunication Network Access to STN
NEWS WWW	CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 12:00:36 ON 26 JUL 2001

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.15	0.15

FILE 'REGISTRY' ENTERED AT 12:01:01 ON 26 JUL 2001

STRUCTURE FILE UPDATES: 25 JUL 2001 HIGHEST RN 348574-08-3
DICTIONARY FILE UPDATES: 25 JUL 2001 HIGHEST RN 348574-08-3

TSCA INFORMATION NOW CURRENT THROUGH January 11, 2001

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Structure search limits have been increased. See HELP SLIMIT for details.

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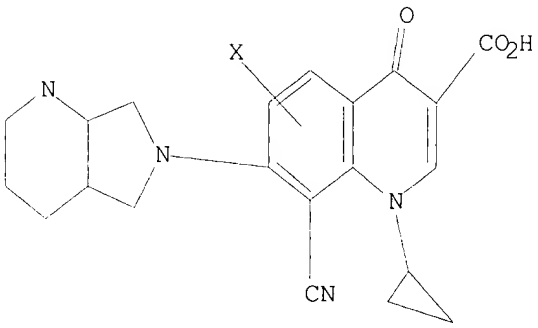
Uploading 09856571.str

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 12:01:44 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 40 TO ITERATE

100.0% PROCESSED 40 ITERATIONS 2 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 421 TO 1179
PROJECTED ANSWERS: 2 TO 124

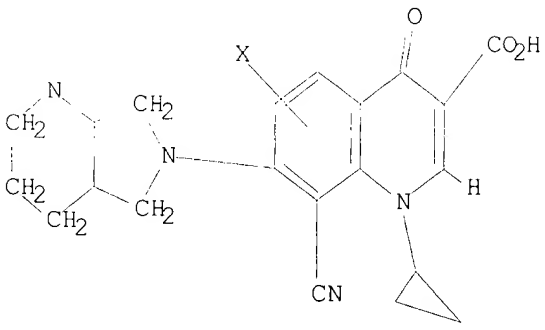
L2 2 SEA SSS SAM L1

=>
Uploading 9856571a.str

L3 STRUCTURE UPLOADED

=> d l3

L3 HAS NO ANSWERS
L3 STR



Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SCREEN SEARCH COMPLETED - 40 TO ITERATE

100.0% PROCESSED 40 ITERATIONS 2 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 421 TO 1179
PROJECTED ANSWERS: 2 TO 124

L4 2 SEA SSS SAM L3

=> s l4 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 133.25 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y

FULL SEARCH INITIATED 12:03:12 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 908 TO ITERATE

100.0% PROCESSED 908 ITERATIONS 18 ANSWERS
SEARCH TIME: 00.00.01

L5 18 SEA SSS FUL L3

=> file ca

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	134.49	134.64

FILE 'CA' ENTERED AT 12:03:19 ON 26 JUL 2001
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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FILE COVERS 1947 - 19 Jul 2001 VOL 135 ISS 5
FILE LAST UPDATED: 19 Jul 2001 (20010719/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

This file supports REG1stRY for direct browsing and searching of all substance data from the REG1STRY file. Enter HELP FIRST for more information.

The CA file now provides online access to patents and literature covered in CA from 1947 to the present. On April 22, 2001, bibliographic information and abstracts were added for over 2.2 million references published in CA from 1947 to 1966.

The CA Lexicon is now available in the Controlled Term (/CT) field. Enter HELP LEXICON for full details.

=> s l5

L6 6 L5

=> s l6 and himmler, t?/au

53 HIMMLER, T?/AU
L7 6 L6 AND HIMMLER, T?/AU

=> s l6 and pd < december 1988

11027737 PD < DECEMBER 1988
(PD<19881200)
L8 0 L6 AND PD < DECEMBER 1988

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=> s l6 and pd < december 1998

      17145426 PD < DECEMBER 1998
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L9            1 L6 AND PD < DECEMBER 1998

=> d l9, ibib abs hitstr, 1
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L9 ANSWER 1 OF 1 CA COPYRIGHT 2001 ACS
ACCESSION NUMBER: 127:248093 CA
TITLE:
8-Cyano-1-cyclopropyl-7-(2,8-diazabicyclo[4.3.0]nonan-

8-yl)-6-fluoro-1,4-dihydro-4-oxo-3-quinolinecarboxylic
acid derivatives
INVENTOR(S): Bartel, Stefan; Jaetsch, Thomas; Himmler, Thomas; Rast, Hans-Georg; Hallenbach, Werner; Heinen, Ernst; Pirro, Franz; Scheer, Martin; Stegemann, Michael; Stupp, Hans-Peter; Wetzstein, Heinz-Georg
PATENT ASSIGNEE(S): Bayer A.-G., Germany; Bartel, Stefan; Jaetsch, Thomas;

Himmler, Thomas; Rast, Hans-Georg; Hallenbach, Werner;

Heinen, Ernst; Pirro, Franz; Scheer, Martin; et al.
SOURCE: PCT Int. Appl., 36 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
WO 9731001	A1	19970828	WO 1997-EP637	19970212	<--
W: AU, BB, BG, BR, BY, CA, CN, CZ, HU, IL, JP, KR, KZ, LK, MX, NO, NZ, PL, RO, RU, SK, TR, UA, US					
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG					
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CA 2247020	AA	19970828	CA 1997-2247020	19970212	<--
AU 9717689	A1	19970910	AU 1997-17689	19970212	<--
AU 715341	B2	20000120			
EP 882049	A1	19981209	EP 1997-903260	19970212	
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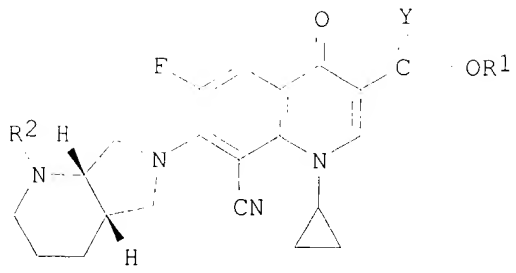
CN 1211984	A	19990324	CN 1997-192523	19970212	
BR 9707606	A	19990727	BR 1997-7606	19970212	
JP 2000504734	T2	20000418	JP 1997-529755	19970212	
NO 9803819	A	19980820	NO 1998-3819	19980820	<--

PRIORITY APPLN. INFO.: DE 1996-19606762 19960223
DE 1996-19633805 19960822
WO 1997-EP637 19970212
OTHER SOURCE(S): MARPAT 127:248093
GI



I

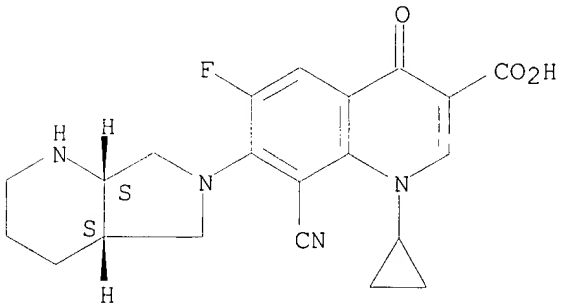
AB Title compds. I [R1 = H, alkyl, optionally substituted by OH, OMe, NH2, NHMe, NMe2, or (5-methyl-2-oxo-1,3-dioxol-4-yl)methyl; R2 = H, benzyl, alkyl, (5-methyl-2-oxo-1,3-dioxol-4-yl)methyl, CH=CHCO2R3, CH2CH2CO2R3, CH2CH2CN, CH2CH2COMe, CH2COMe; R3 = Me, Et, R4(NHCHR5CO)n; R4 = H, alkyl, CO2CMe3; R5 = H, alkyl, hydroxyalkyl, aminoalkyl, thioalkyl, carboxyalkyl, benzyl; n = 1, 2; Y = O, S] were prepd. for use as antibacterial agents. Thus, I [R1 = OH, R2 = H, Y = O] was prepd. by aminating the 7-chloroquinoline. I [R1 = OH, R2 = H, Y = O] had min. inhibitory concns. against a no. of bacteria that were superior to those of enrofloxacin.

IT **195532-12-8P**
RL: BAC (Biological activity or effector, except adverse); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of diazabicylononylquinolinecarboxylic acid derivs. as bactericides)

RN 195532-12-8 CA

CN 3-Quinolinecarboxylic acid, 8-cyano-1-cyclopropyl-6-fluoro-1,4-dihydro-7-[(4aS,7aS)-octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl]-4-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

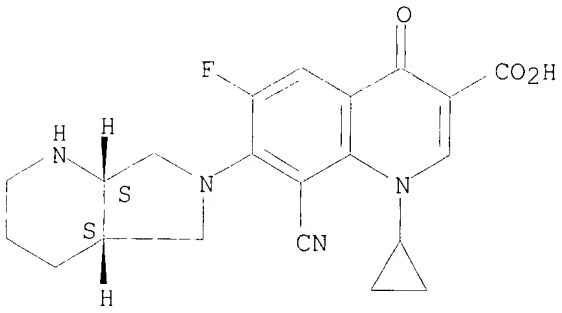


IT **195532-14-0P 195532-16-2P 195532-18-4P**
195532-20-8P 195532-22-0P 195532-25-3P
195532-27-5P 195532-29-7P 195532-31-1P
195532-33-3P 195532-36-6P 195532-39-9P
195532-42-4P 195532-45-7P 195532-48-0P

195532-58-2P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of diazabicylononylquinolinecarboxylic acid derivs. as bactericides)

RN 195532-14-0 CA
CN 3-Quinolinecarboxylic acid, 8-cyano-1-cyclopropyl-6-fluoro-1,4-dihydro-7-(octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl)-4-oxo-, monohydrochloride, (4aS-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



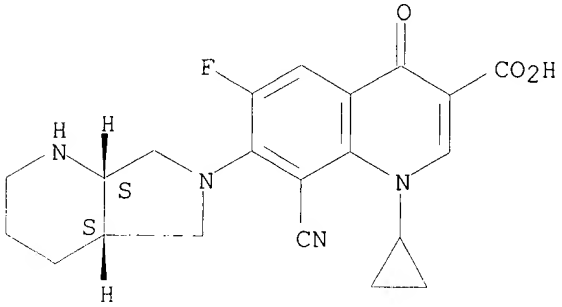
● HCl

RN 195532-16-2 CA
CN 3-Quinolinecarboxylic acid, 8-cyano-1-cyclopropyl-6-fluoro-1,4-dihydro-7-(octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl)-4-oxo-, (4aS-cis)-, monomethanesulfonate (9CI) (CA INDEX NAME)

CM 1

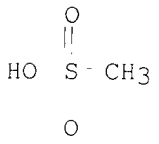
CRN 195532-12-8
CMF C21 H21 F N4 O3

Absolute stereochemistry.



CM 2

CRN 75-75-2
CMF C H4 O3 S

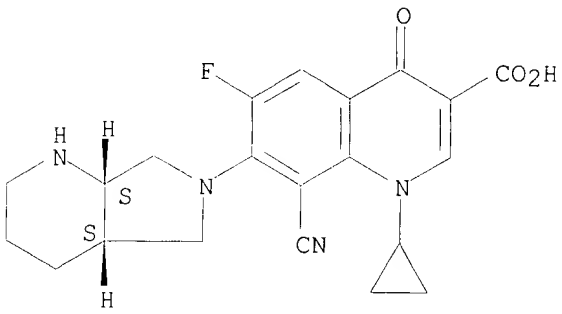


RN 195532-18-4 CA
CN 3-Quinolinecarboxylic acid, 8-cyano-1-cyclopropyl-6-fluoro-1,4-dihydro-7-(octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl)-4-oxo-, (4aS-cis)-, mono(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

CM 1

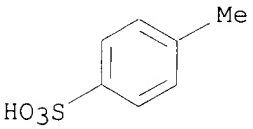
CRN 195532-12-8
CMF C21 H21 F N4 O3

Absolute stereochemistry.



CM 2

CRN 104-15-4
CMF C7 H8 O3 S

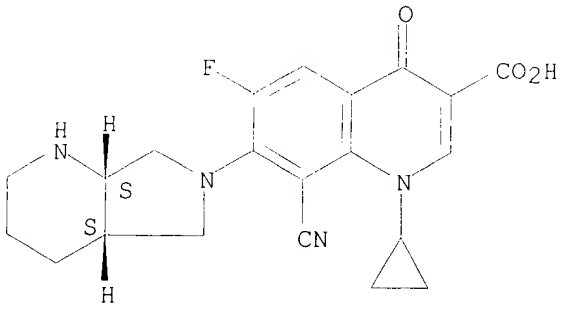


RN 195532-20-8 CA
CN 3-Quinolinecarboxylic acid, 8-cyano-1-cyclopropyl-6-fluoro-1,4-dihydro-7-(octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl)-4-oxo-, (4aS-cis)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

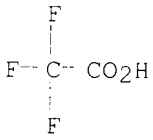
CRN 195532-12-8
CMF C21 H21 F N4 O3

Absolute stereochemistry.



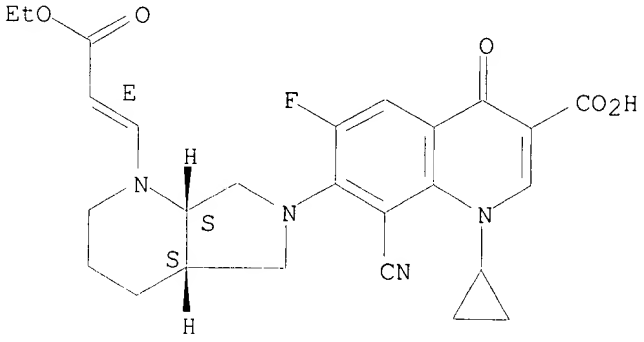
CM 2

CRN 76-05-1
CMF C2 H F3 O2



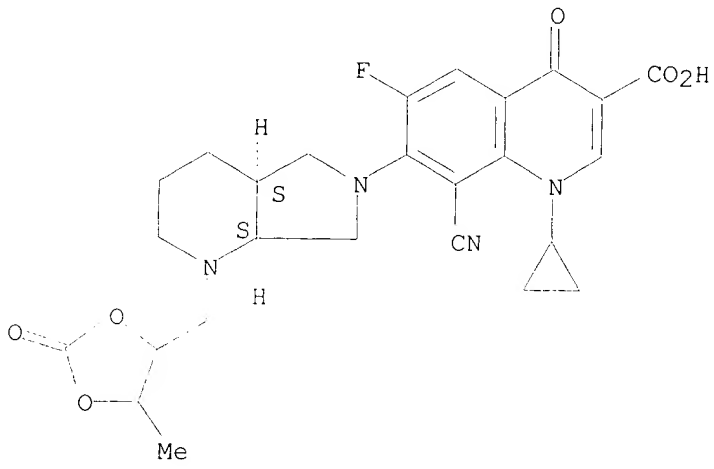
RN 195532-22-0 CA
CN 3-Quinolinecarboxylic acid, 8-cyano-1-cyclopropyl-7-[1-(3-ethoxy-3-oxo-1-propenyl)octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl]-6-fluoro-1,4-dihydro-4-oxo-, [4aS-[1(E),4a.alpha.,7a.alpha.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 195532-25-3 CA
CN 3-Quinolinecarboxylic acid, 8-cyano-1-cyclopropyl-6-fluoro-1,4-dihydro-7-[octahydro-1-[(5-methyl-2-oxo-1,3-dioxolan-4-yl)methyl]-6H-pyrrolo[3,4-b]pyridin-6-yl]-4-oxo-, [4aS-(4a.alpha.,7a.alpha.)]-[partial]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 195532-27-5 CA
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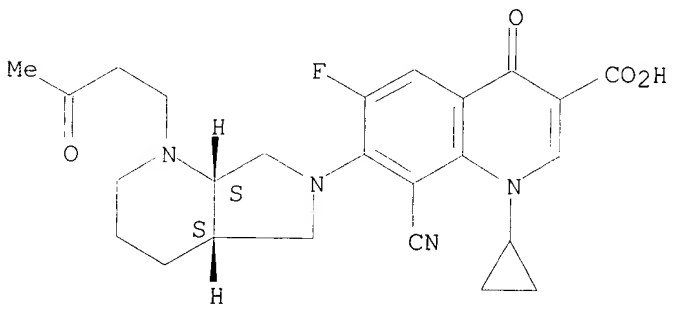
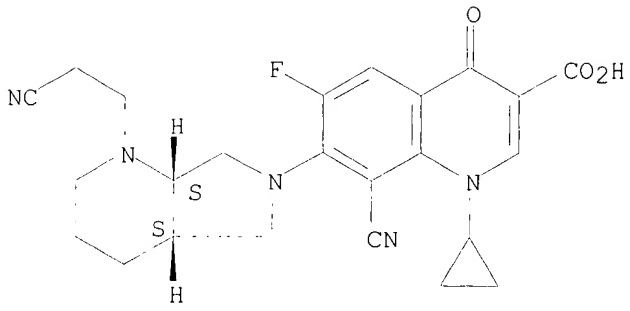
Absolute stereochemistry.



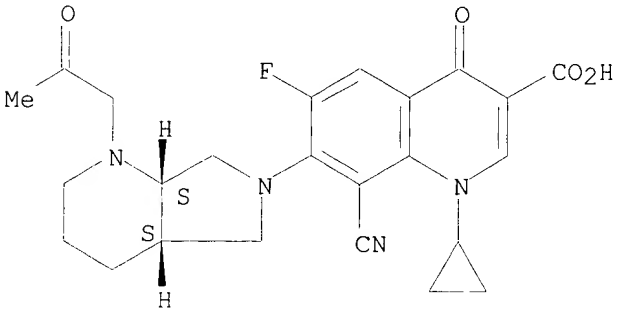
RN 195532-29-7 CA
CN 3-Quinolinecarboxylic acid, 8-cyano-7-[1-(2-cyanoethyl)octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl]-1-cyclopropyl-6-fluoro-1,4-dihydro-4-oxo-, (4aS-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



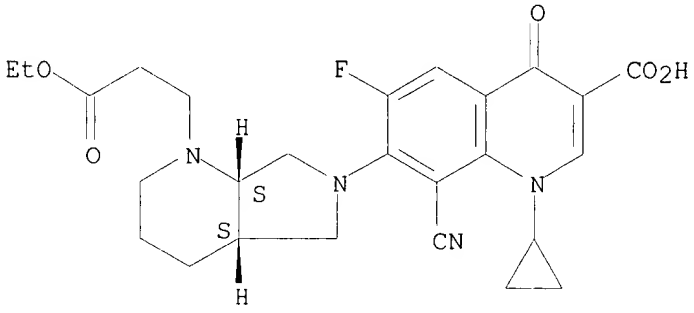
RN 195532-31-1 CA
CN 3-Quinolinecarboxylic acid, 8-cyano-1-cyclopropyl-6-fluoro-1,4-dihydro-7-[octahydro-1-(2-oxopropyl)-6H-pyrrolo[3,4-b]pyridin-6-yl]-4-oxo-, (4aS-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 195532-33-3 CA
CN 3-Quinolinecarboxylic acid, 8-cyano-1-cyclopropyl-7-[1-(3-ethoxy-3-oxopropyl)octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl]-6-fluoro-1,4-dihydro-4-oxo-, (4aS-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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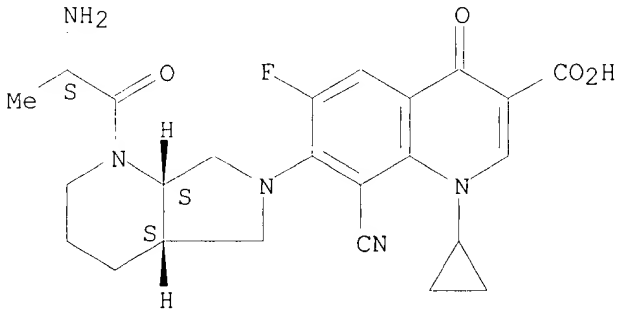
pyrrolo[3,4-b]pyridin-6-yl]-8-cyano-1-cyclopropyl-6-fluoro-1,4-dihydro-4-oxo-, monohydrochloride, [4aS-[1(R*),4a.alpha.,7a.alpha.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● HCl

RN 195532-39-9 CA
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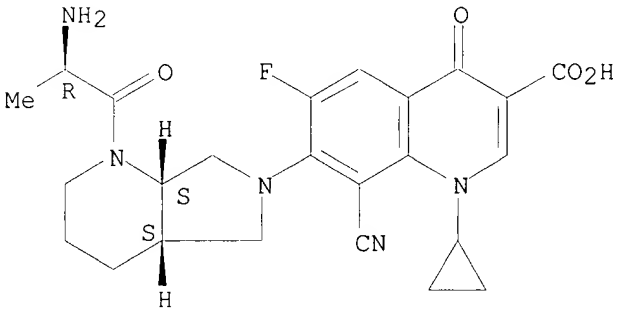
Absolute stereochemistry.



● HCl

RN 195532-42-4 CA
CN 3-Quinolinecarboxylic acid,
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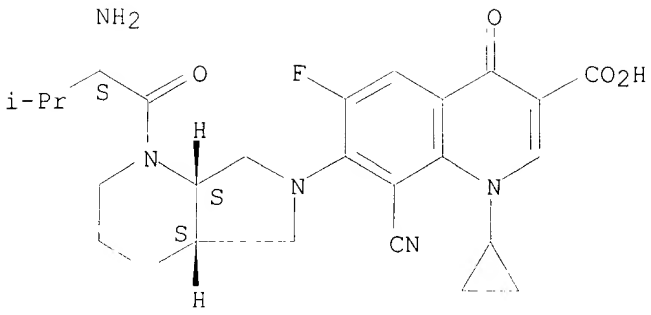
Absolute stereochemistry.



● HCl

RN 195532-45-7 CA
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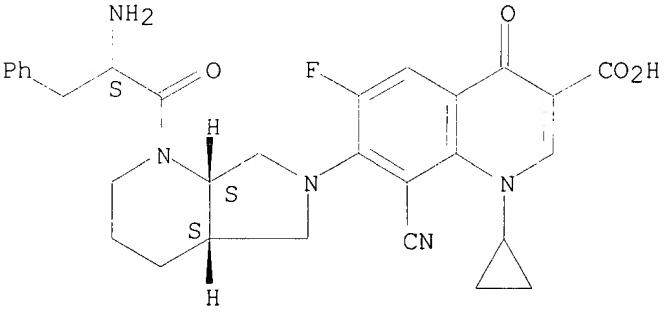
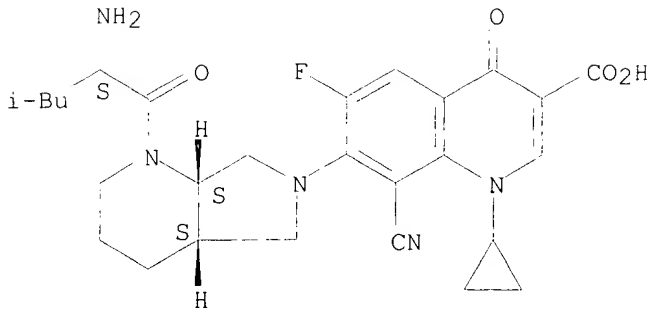
Absolute stereochemistry.



● HCl

RN 195532-48-0 CA
CN 3-Quinolinecarboxylic acid, 7-[1-(2-amino-4-methyl-1-oxopentyl)octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl]-8-cyano-1-cyclopropyl-6-fluoro-1,4-dihydro-4-oxo-, monohydrochloride, [4aS-[1(R*),4a.alpha.,7a.alpha.]]- (9CI) (CA INDEX NAME)

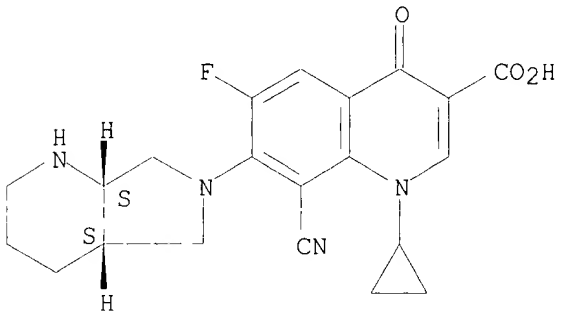
Absolute stereochemistry.



● HCl

RN 195532-58-2 CA
CN 3-Quinolinecarboxylic acid, 8-cyano-1-cyclopropyl-6-fluoro-1,4-dihydro-7-(octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl)-4-oxo-, monosodium salt, (4aS-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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L5 18 S L4 FULL

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L6              6 S L5
L7              6 S L6 AND HIMMLER, T?/AU
L8              0 S L6 AND PD < DECEMBER 1988
L9              1 S L6 AND PD < DECEMBER 1998

=> s l6 not l9

L10             5 L6 NOT L9

=> d l10, ibib abs fhitstr, 1-5


L10  ANSWER 1 OF 5  CA  COPYRIGHT 2001 ACS
ACCESSION NUMBER:         133:213147  CA
TITLE:                    Crystal modification C of 8-cyano-1-cyclopropyl-7-
                          [(1S,6S)-2,8-diazabicyclo[4.3.0]nonan-8-yl]-6-fluoro-
                          1,4-dihydro-4-oxo-3-quinolinecarboxylic acid
INVENTOR(S):              Rast, Hubert; Himmler, Thomas
PATENT ASSIGNEE(S):       Bayer A.-G., Germany
SOURCE:                   Ger. Offen., 12 pp.
                          CODEN: GWXXBX
DOCUMENT TYPE:            Patent
LANGUAGE:                 German
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.        KIND  DATE           APPLICATION NO.   DATE
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     DE 19908449        A1   20000831       DE 1999-19908449 19990226
     WO 2000052009      A1   20000908       WO 2000-EP1202   20000214
         W:  AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU,
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             IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA,
             MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI,
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             AZ, BY, KG, KZ, MD, RU, TJ, TM
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PRIORITY APPLN. INFO.:                  DE 1999-19908449 A  19990226
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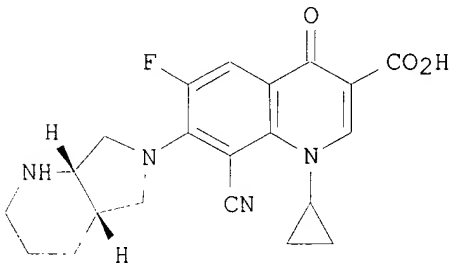


I

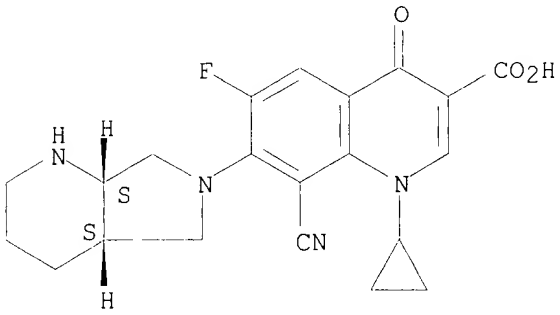
AB The title compd. (I) is converted to stable crystal modification C (m. 235-237.degree.) by holding I at room temp. and relative humidity .gtoreq.92% until no further wt. gain occurs, drying, and heating to above the conversion temp. (150-180.degree.). I modification D is characterized by its powder x-ray diffractogram, IR spectrum, and by DTA. I is highly active against pathogenic bacteria in human and veterinary medicine.

IT **195532-12-8**
RL: BAC (Biological activity or effector, except adverse); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(crystal modification D of cyanocyclopropyl(diazabicyclononanyl)fluorodihydrooxoquinolinecarboxylic acid)

RN 195532-12-8 CA

CN 3-Quinolinecarboxylic acid, 8-cyano-1-cyclopropyl-6-fluoro-1,4-dihydro-7-[(4aS,7aS)-octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl]-4-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L10 ANSWER 2 OF 5 CA COPYRIGHT 2001 ACS
ACCESSION NUMBER: 133:213146 CA
TITLE: Crystal modification D of 8-cyano-1-cyclopropyl-7-[(1S,6S)-2,8-diazabicyclo[4.3.0]nonan-8-yl]-6-fluoro-1,4-dihydro-4-oxo-3-quinolinecarboxylic acid
INVENTOR(S): Himmler, Thomas; Rast, Hubert
PATENT ASSIGNEE(S): Bayer A.-G., Germany
SOURCE: Ger. Offen., 12 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19908448	A1	20000831	DE 1999-19908448	19990226
WO 2000052010	A1	20000908	WO 2000-EP1203	20000214

W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL,

IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA,
MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI,
SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM,
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RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,
DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,
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PRIORITY APPLN. INFO.: DE 1999-19908448 A 19990226
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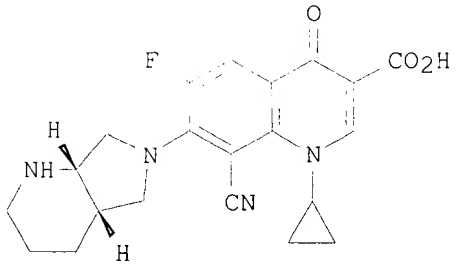


I

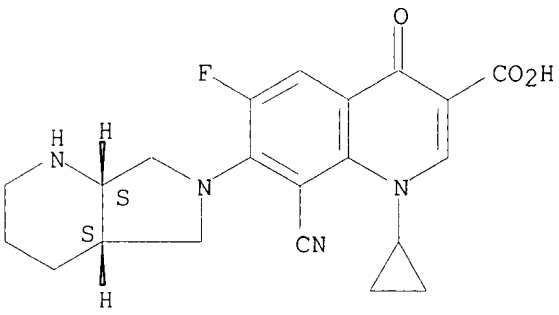
AB The title compd. (I) is converted to stable crystal modification D (m. 261-265.degree.) by dissolving I in H2O to a concn. of 1-3 wt.%, allowing the soln. to stand until a ppt. forms, removing the ppt. by filtration, drying the remaining soln., and heating the solid obtained to above the transition temp. (130-160.degree.). I modification D is characterized by its powder x-ray diffractogram, IR spectrum, and by DTA. I is highly active against pathogenic bacteria in human and veterinary medicine.

IT **195532-12-8**
RL: BAC (Biological activity or effector, except adverse); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(crystal modification D of cyanocyclopropyl(diazabicyclononanyl)fluorodihydrooxoquinolinecarboxylic acid)

RN 195532-12-8 CA

CN 3-Quinolinecarboxylic acid, 8-cyano-1-cyclopropyl-6-fluoro-1,4-dihydro-7-[(4aS,7aS)-octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl]-4-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L10 ANSWER 3 OF 5 CA COPYRIGHT 2001 ACS
ACCESSION NUMBER: 133:4647 CA
TITLE: Semihydrochloride of 8-cyano-1-cyclopropyl-7-(1S,6S-2,8-diazabicyclo[4.3.0]nonan-8-yl)-6-fluoro-1,4-dihydro-4-oxo-3-quinolinecarboxylic acid
INVENTOR(S): Himmler, Thomas; Rast, Hubert
PATENT ASSIGNEE(S): Bayer A.-G., Germany
SOURCE: Ger. Offen., 16 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19854357	A1	20000531	DE 1998-19854357	19981125
WO 2000031077	A1	20000602	WO 1999-EP8778	19991115

W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: DE 1998-19854357 A 19981125
OTHER SOURCE(S): CASREACT 133:4647
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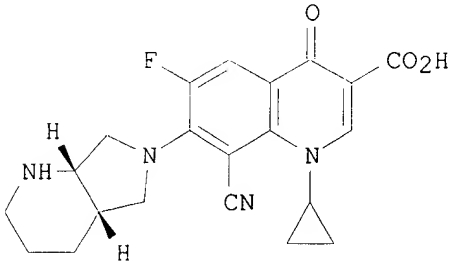


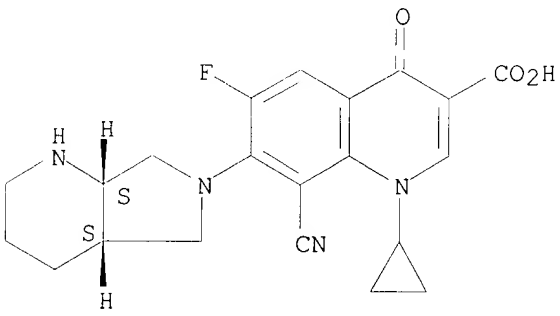
ClH
1/2 HCl

I

AB The title compd. (I), useful as a medical and veterinary bactericide, shows good water soly. (19 wt.%). I is produced by reaction of 7-halo-8-cyano-1-cyclopropyl-6-fluoro-1,4-dihydro-4-oxo-3-quinolinecarboxylic acid with (1S,6S)-2,8-diazabicyclo[4.3.0]nonane in the presence of a base in one of the following diluents: (a) a C.gtoreq.4 aliph. alc., (b) a mixt. of a C>3 alc. with the polar aprotic diluent, N-methylpyrrolidone; (c) a mixt. of n-PrOH with DMF. I (m. 278-280.degree.) is characterized by its powder x-ray diffractogram, differential thermogram, and IR spectrum.

IT **271252-05-2P**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN
(Synthetic preparation); PREP (Preparation); PROC (Process)
(semihydrochloride of cyanocyclopropyl(diazabicyclononyl)fluorodihydrooxoquinolinecarboxylic acid)
RN 271252-05-2 CA
CN 3-Quinolinecarboxylic acid, 8-cyano-1-cyclopropyl-6-fluoro-1,4-dihydro-7-[(4aS,7aS)-octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl]-4-oxo-, hydrochloride (2:1) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● 1/2 HCl

L10 ANSWER 4 OF 5 CA COPYRIGHT 2001 ACS
ACCESSION NUMBER: 133:4646 CA
TITLE: Crystal modification A of 8-cyano-1-cyclopropyl-7-(1S,6S-2,8-diazabicyclo[4.3.0]nonan-8-yl)-6-fluoro-1,4-dihydro-4-oxo-3-quinolinecarboxylic acid
INVENTOR(S): Himmler, Thomas; Hallenbach, Werner; Rast, Hubert
PATENT ASSIGNEE(S): Bayer A.-G., Germany
SOURCE: Ger. Offen., 8 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19854356	A1	20000531	DE 1998-19854356	19981125
WO 2000031075	A1	20000602	WO 1999-EP8775	19991115

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AZ, BY, KG, KZ, MD, RU, TJ, TM
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PRIORITY APPLN. INFO.: DE 1998-19854356 A 19981125
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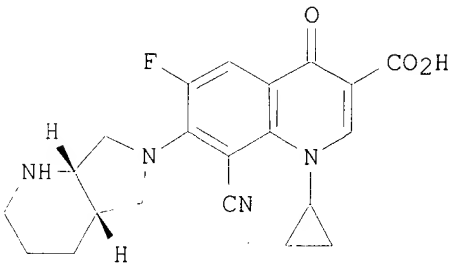


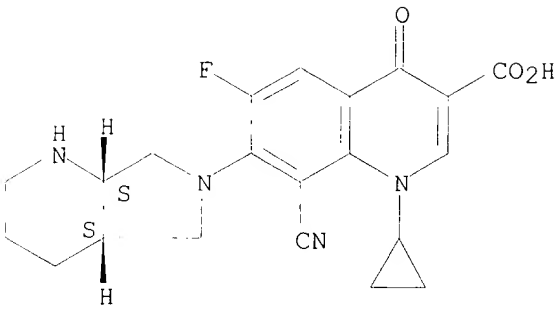
I

AB The title compd. in crystal modification A (I), useful as a medical and veterinary bactericide, is stable during extended storage without conversion to the amorphous form or any other crystal modification, and is less hygroscopic than the amorphous form of the compd. I is produced by dissolving the amorphous compd. or an unknown modification of it in hot water or a hot water-alc. mixt., adding an alc. (esp. EtOH or iso-PrOH), and cooling to room temp. I (m. 249-252.degree.) is characterized by its powder x-ray diffractogram, differential thermogram, and IR spectrum.

IT **195532-12-8P**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(crystal modification A of cyanocyclopropyl(diazabicyclononyl)fluorodihydrooxoquinolinecarboxylic acid)

RN 195532-12-8 CA
CN 3-Quinolinecarboxylic acid, 8-cyano-1-cyclopropyl-6-fluoro-1,4-dihydro-7-[(4aS,7aS)-octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl]-4-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L10 ANSWER 5 OF 5 CA COPYRIGHT 2001 ACS
ACCESSION NUMBER: 133:4645 CA
TITLE: Crystal modification B of 8-cyano-1-cyclopropyl-7-(1S,6S-2,8-diazabicyclo[4.3.0]nonan-8-yl)-6-fluoro-1,4-dihydro-4-oxo-3-quinolinecarboxylic acid
INVENTOR(S): Himmler, Thomas; Hallenbach, Werner; Rast, Hubert
PATENT ASSIGNEE(S): Bayer A.-G., Germany
SOURCE: Ger. Offen., 8 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2000031076	A1	20000602	WO 1999-EP8776	19991115

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PRIORITY APPLN. INFO.: DE 1998-19854355 A 19981125
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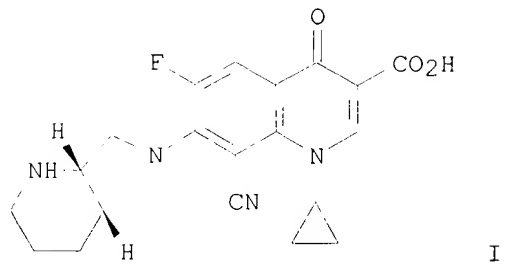


I

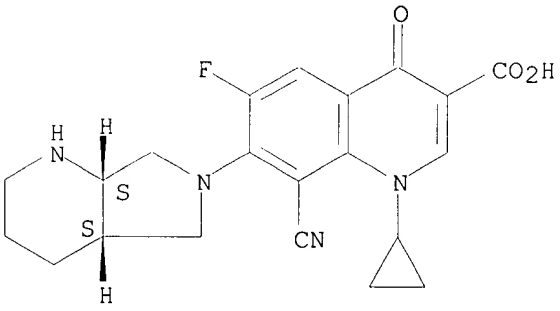
AB The title compd. in crystal modification B (I), useful as a medical and veterinary bactericide, is stable during extended storage without conversion to the amorphous form or any other crystal modification, and is less hygroscopic than the amorphous form of the compd. I is produced either (a) by reaction of 7-halo-8-cyano-1-cyclopropyl-6-fluoro-1,4-dihydro-4-oxo-3-quinolinecarboxylic acid with (1S,6S)-2,8-diazabicyclo[4.3.0]nonane in the presence of a base in a mixt. of EtOH and a polar aprotic diluent such as N-methylpyrrolidone, DMF, or sulfolane, or (b) by heating an unknown modification of the compd. in the presence of a base in EtOH, n-PrOH, iso-PrOH, or a mixt. of one of these alcs. with one of the polar aprotic diluents named previously. I (m. 243-245.degree.) is characterized by its powder x-ray diffractogram, differential thermogram, and IR spectrum.

IT **195532-12-8P**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(crystal modification B of cyanocyclopropyl(diazabicyclononyl)fluorodihydrooxoquinolinecarboxylic acid)

RN 195532-12-8 CA

CN 3-Quinolinecarboxylic acid, 8-cyano-1-cyclopropyl-6-fluoro-1,4-dihydro-7-[(4aS,7aS)-octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl]-4-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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FILE 'CAOLD' ENTERED AT 12:06:02 ON 26 JUL 2001
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FILE COVERS 1907-1966
FILE LAST UPDATED:  01 May 1997 (19970501/UP)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.  Title keywords, authors, patent
  assignees, and patent information, e.g., patent numbers, are
  now searchable from 1907-1966.  TIFF images of CA abstracts
  printed between 1907-1966 are available in the PAGE
  display formats.

  This file supports REG1stRY for direct browsing and searching of
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  more information.

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     (FILE 'HOME' ENTERED AT 12:00:36 ON 26 JUL 2001)

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L9           1 S L6 AND PD < DECEMBER 1998
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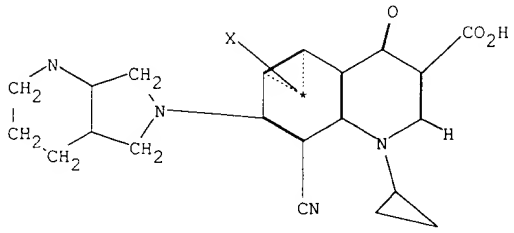

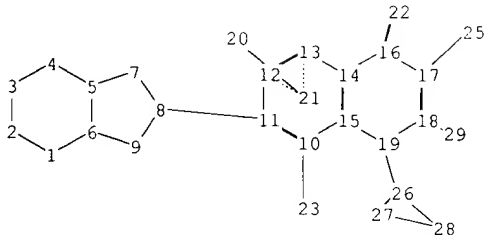

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ring nodes :
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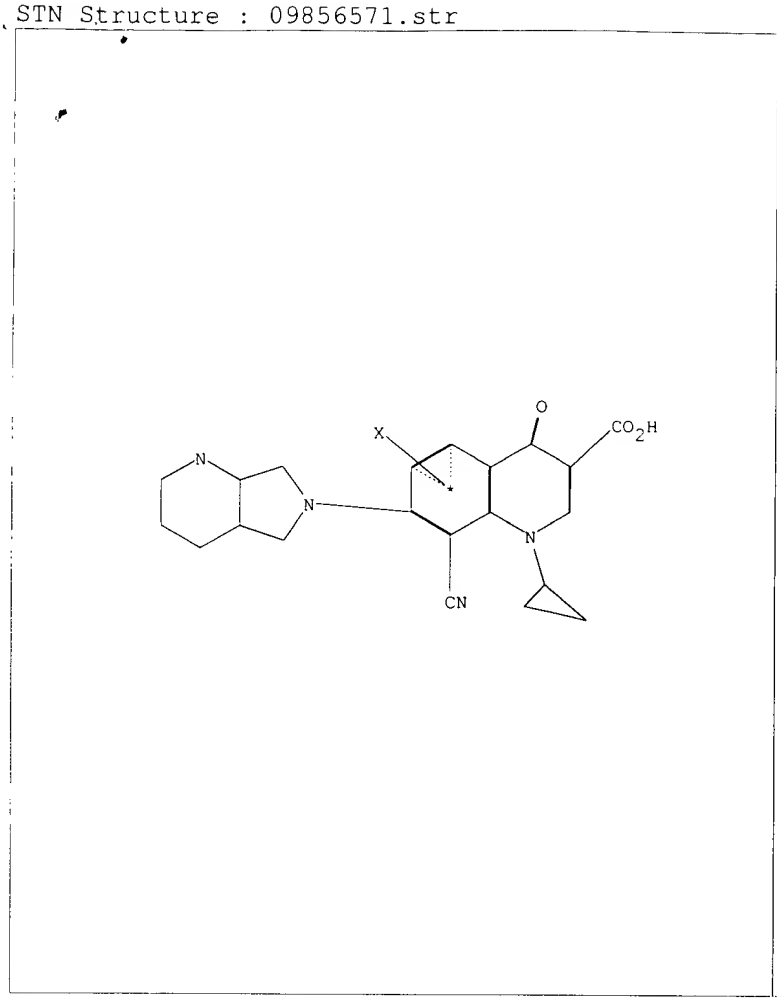
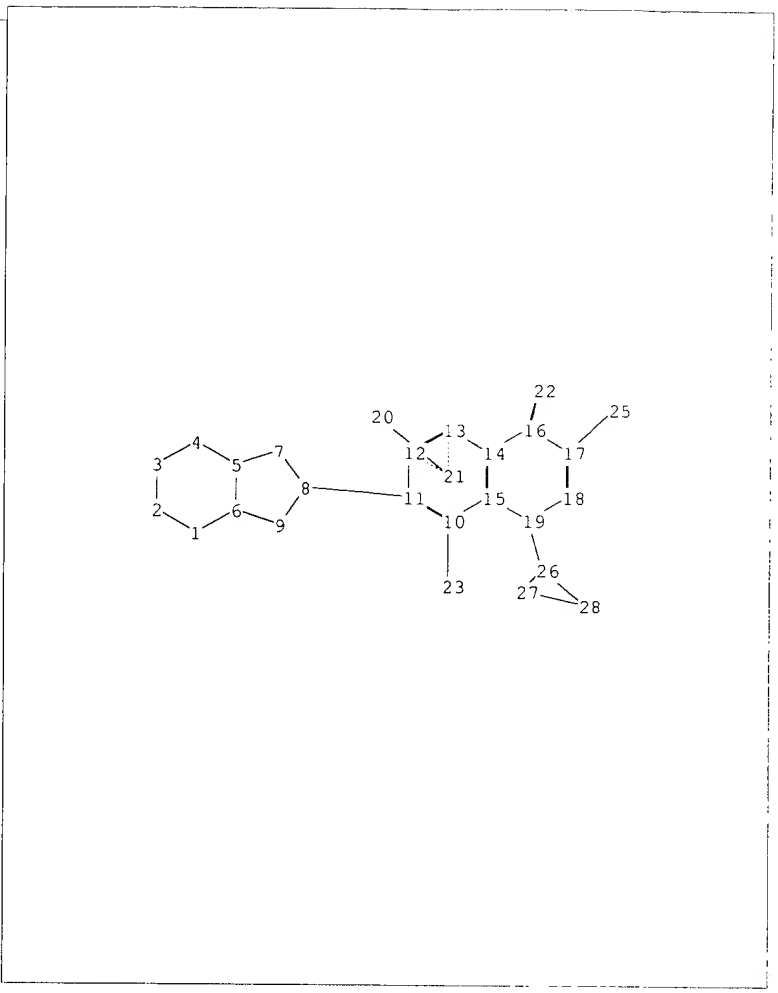
chain bonds :
8-11 10-23 16-22 17-25 18-29 19-26
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 10-11 10-15 11-12 12-13 13-14
14-15 14-16 15-19 16-17 17-18 18-19 26-27 26-28 27-28
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 5-6 8-11 14-16 15-19 16-17 16-22 17-18 18-19 19-26
26-27 26-28 27-28
exact bonds :
5-7 6-9 7-8 8-9 10-23 17-25 18-29
normalized bonds :
10-11 10-15 11-12 12-13 13-14 14-15
isolated ring systems :
containing 1 : 10 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:CLASS
21:CLASS 22:CLASS 23:CLASS 25:CLASS 26:Atom 27:Atom 28:Atom 29:CLASS

STN Structure : 09856571.str





chain nodes :
20 22 23 25
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 26 27 28
chain bonds :
8-11 10-23 16-22 17-25 19-26
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 10-11 10-15 11-12 12-13 13-14
14-15 14-16 15-19 16-17 17-18 18-19 26-27 26-28 27-28
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 8-9 8-11 14-16 15-19 16-17 16-22 17-18 18-19
19-26 26-27 26-28 27-28
exact bonds :
5-7 6-9 10-23 17-25
normalized bonds :
10-11 10-15 11-12 12-13 13-14 14-15
isolated ring systems :
containing 1 : 10 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:CLASS
21:CLASS 22:CLASS 23:CLASS 25:CLASS 26:Atom 27:Atom 28:Atom

```
=> d his

     (FILE 'HOME' ENTERED AT 12:00:36 ON 26 JUL 2001)

     FILE 'REGISTRY' ENTERED AT 12:01:01 ON 26 JUL 2001
L1             STRUCTURE UPLOADED
L2           2 S L1
L3             STRUCTURE UPLOADED
L4           2 S L3
L5          18 S L4 FULL

     FILE 'CA' ENTERED AT 12:03:19 ON 26 JUL 2001
L6           6 S L5
L7           6 S L6 AND HIMMLER, T?/AU
L8           0 S L6 AND PD < DECEMBER 1988
L9           1 S L6 AND PD < DECEMBER 1998
L10          5 S L6 NOT L9

     FILE 'CAOLD' ENTERED AT 12:06:02 ON 26 JUL 2001

=> s l5

L11          0 L5
```